Annual Reports 1993-94

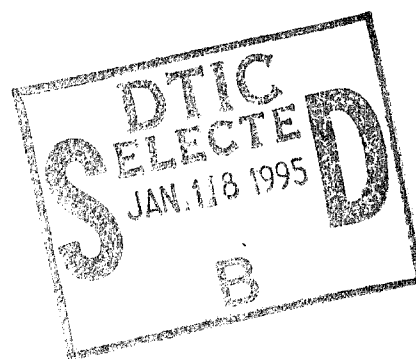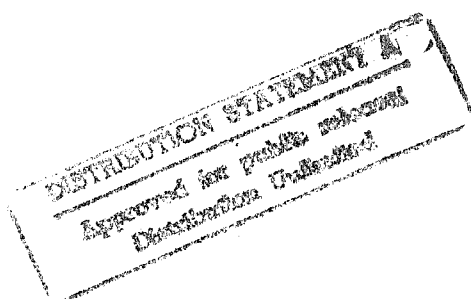## ONR Grant N00014-92-1284

Predicting Polarized Light Scattering by Marine Micro-Organisms

Principal Investigator: Patricia G. Hull

Tennessee State University

Department of Physics, Mathematics and Computer Science

March 1, 1992 to February 28, 1994

19950113 030

Predicting Polarized Light Scattering from Marine Micro-organisms

Patricia G. Hull
Tennessee State University
Department of Physics and Mathematics
3500 John Merritt Blvd.
Nashville, TN 37209-1561
Phone/FAX: 615-963-5846
e-mail address: phull@acad.tnstate.edu

DTIC
S ELECTED
JAN 1|8 1995
B
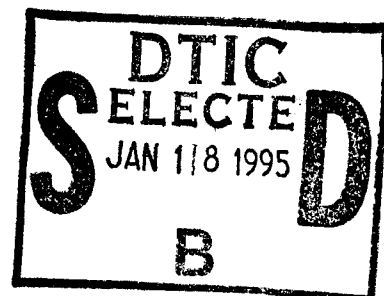
Research Goals

To understand and quantify light scattering from ensembles of irregularly-shaped objects. To characterize the effect of ensembles of micro-organisms on the propagation of polarized light through sea water. To determine the feasibility of detecting particle orientation and to assess the importance of scattering to underwater imaging techniques and irradiance calculations.

Objectives

To develop a numerical or analytical model that predicts angle-dependent scattering of polarized light from ensembles of non-spherical marine organisms and marine detritus.   To verify and examine the validity and range of applications of the model by comparison with exact calculations and/or experimental results as appropriate.   To apply the model to investigate the effects caused by the orientation of ensembles of non-spherical particles, and to determine the feasibility of detecting orientation by measuring scattering matrix elements that are normally zero.

Approach

The polarization states of the incident and scattered light are described by four-element vectors called Stokes vectors. The effect of the scattering medium on the incident beam is described by a sixteen-element matrix called the Mueller or scattering matrix. The elements of the scattering matrix depend on the scattering angle and contain all the elastic scattering information available at a given wavelength. They are functions of the size, structure, symmetry, orientation, complex refractive index, and ordering of the scatterers.

The coupled-dipole approximation is used to model the micro-organisms. In this model, an arbitrarily-shaped object is divided into a number of identical elements arranged on a cubic lattice. For isotropic materials, each element is treated as a spherical, dipolar oscillator with a scalar polarizability. The anisotropy of a material is described by using ellipsoidal polarizability tensors at each dipole
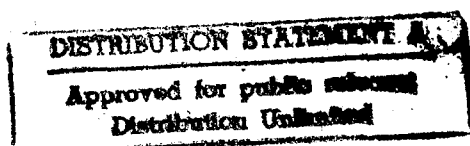
site. Interactions between dipoles are included by determining the field at a particular dipole due to the incident field and the fields induced by the other dipole oscillators. The scattered field is then the sum of the fields due to each oscillator. The Mueller matrix elements are calculated from the components of the scattered field.

A model for light scattering that included a method of representing a collection of organisms was developed. A reasonable approach is to perform a numerical or analytical average over a set of orientations of a single particle by rotating its principal axes through the Euler angles. The resulting Mueller matrix elements are assumed to be equivalent to the Mueller matrix elements for light scattered by a collection of randomly oriented particles. Since the integration over the Euler angles is cumbersome and generally inefficient, we chose to fix the particle at one orientation and rotate the coordinate system. Both incident radiation and the scattering plane are expressed in the rotated coordinate system for each orientation, but the large interaction matrix that results from considering interactions between the dipoles is only inverted once. This averaging process adds computation time to the calculations for a single particle but no additional memory is required. All computations using the coupled-dipole model were done on the Naval Oceanography Program's Cray Y-MP8.

Tasks Completed in 1993

The computer code written previously for calculating the sixteen elements of the Mueller scattering matrix for a single object at one orientation was extended to include a routine for averaging the matrix elements over all possible orientations of the particle. This orientation averaging of the matrix elements was accomplished by a three dimensional integration over Euler angles. The integrals were evaluated using Gaussian-Legendre integration. Particles of various shapes including spheres, cylinders, prolate and oblate spheroids, hexagonal disks, single helices, and plectonemic helices similar to the DNA molecule were modeled by collections of spherical, prolate or oblate spheroidal dipoles. Spherical particles were modeled so that comparisons could be made with Mie theory to assess limitations and ranges of application for the coupled-dipole calculations.

Results in 1993

A first Born approximation for modeling a thin wire helix was extended to include the calculation of all the Mueller matrix elements by D. Shapiro at LBL. Comparisons of Mueller matrices for scattering from a single helix calculated by the two methods show good agreement. Calculations of Mueller matrix elements for an ensemble of randomly oriented helices based on the first Born approximation and on coupled-dipole theory were also compared to data taken from octopus sperm. Although micrographs of octopus sperm show a helical shape, experimental measurements of Mueller matrix elements did not agree

well with scattering expected from a helix. On the other hand, dinoflagallates have no overall helical shape, but experimental measurements of light scattering from these organisms are consistent with scattering predicted for a helix, *i.e.* the S_{14} matrix element as a function of scattering angle is non-zero. A possible candidate for the scatterer is the DNA molecule. In order to understand the nature of the scattering from a chiral molecule such as DNA, a model of a plectonemic helix was made using the Couple-Dipole approach. Two examples of the shapes studied are are shown in Figure 1. Results of calculations are shown in Figures 2, 3 and 4. Table 1 below shows the strengths of the polarizabilities in $Å^3$, obtained using absorption data and Kramer-Kronig relations. These activities were in collaboration with A.J. Hunt, M.S. Quinby-Hunt, and D. Shapiro of Lawrence Berkeley Laboratory.

| Wavelength	α_{tt}	α_{nn}	α_{pp}
6330Å	12.8	44	44
2600Å	15.2+0.88i	48.8+36.8i	48.8+36.8i
200Å	0.72+0.4i	0.72+0.4i	0.72+0.4i

Table 1. Components of Polarizability Tensor for three eavelengths. A base pair is represented by a single point polarizable group. The polarizability was cal;culated paralled and perpendicular to the base pair plane using the average absorption of each nucleotide.

Accomplishments in 1993

To date, no model has predicted Mueller matrix elements that compare well to experimental measurements of the scattering from asymmetric ensembles of particles. In a previous section, we discussed progress toward that goal. An increased understanding of the scattering from irregularly-shaped particles has gained by the effort and results of the previous year has, at least, brought us closer to that model.
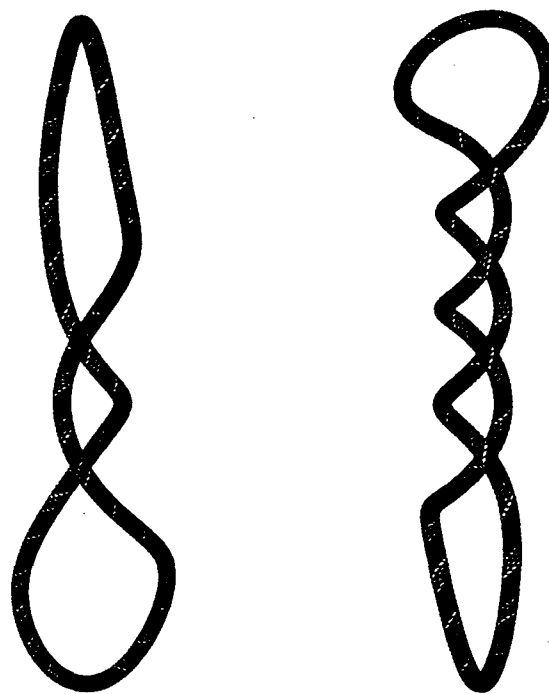
Figure 1. The two (left) and four (right) turn helix

S11

S11

S13

S14

S34

S34
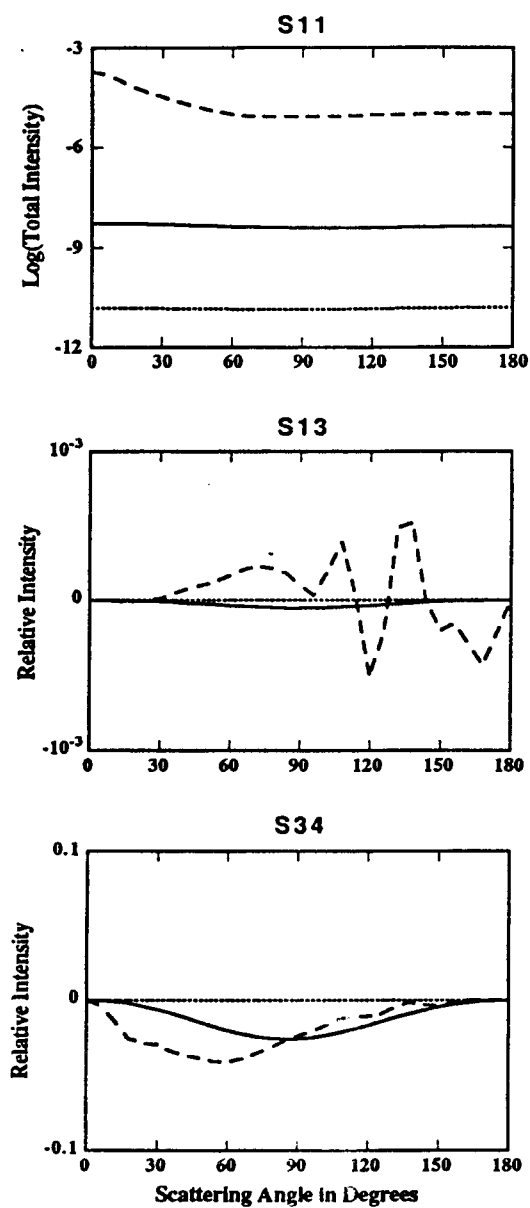
Figure 2. Mueller matrix elements calculated for the two turn helix as a function of wavelength. ···, 6330Å; ——, 2600Å; - - -, 200Å.
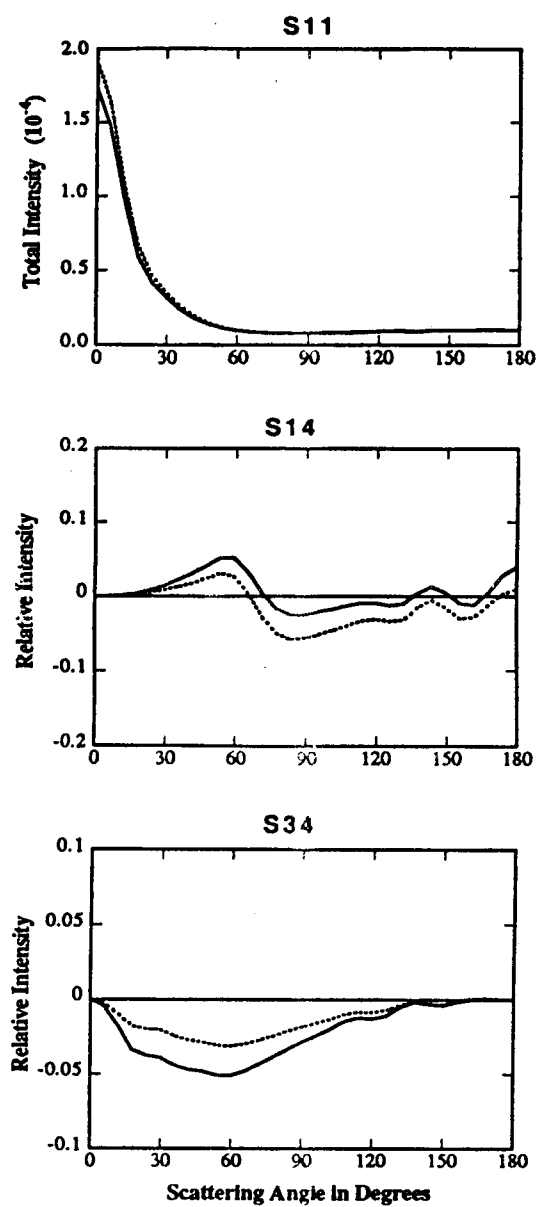
Figure 3. Anisotropic polarizabilities. Perpendicular polarizibilities (---) and parallel polarizabilities (···). The wavelength is 200Å.
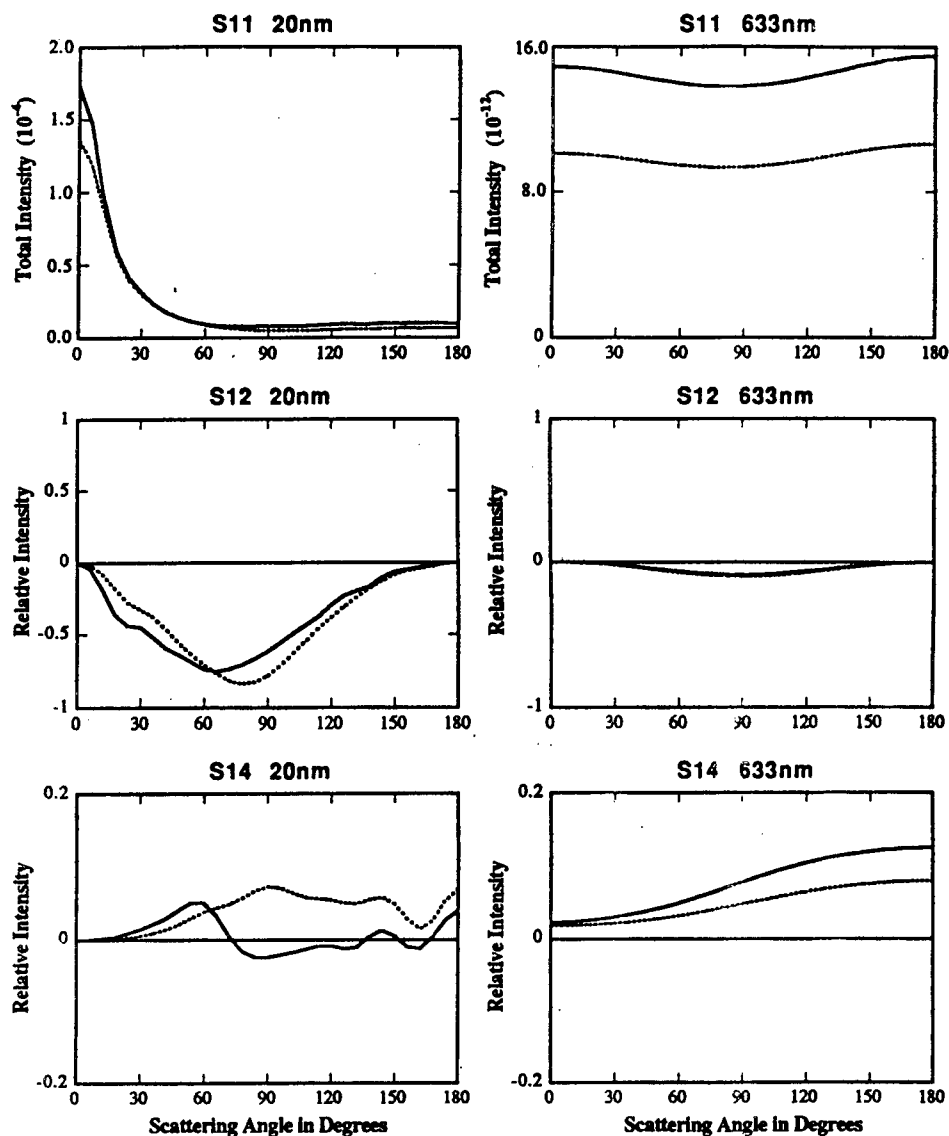
Figure 4. The writhe dependence of the Mueller matrix elements. The matrix elements, normalized by S11, are plotted vs. scattering angle for the two(——) and four (····) turn helices. The polarizability strengths at each wavelength are shown in Table 1.

Tasks Completed in 1994

The development of computer codes for calculating the sixteen elements of the Mueller scattering matrix for a collection of randomly oriented particles was completed. The computer programs were written to allow for modeling of a particle with dipoles of isotropic or anisotropic polarizabilities. An analytical solution for the orientational average based on the rotational properties of spherical tensors served as a guide to evaluate various approximation methods. Unfortunately, the computer memory required to carry out the calculation of the analytical solutions was prohibitive for particles modeled by a large number of dipoles. Several approximation methods were examined including Monte-Carlo, Romberg, and Gaussian-Legendre integration. The orientational average using Gaussian-Legendre integration proved to converge more rapidly than other methods examined when compared to the analytical calculations. Particles of various shapes including cylinders, cubes, prolate spheroids, hexagonal disks and helices were modeled by collections of dipoles. Spherical particles were also modeled so that comparisons could be made with Mie theory to assess limitations and ranges of application for the coupled-dipole calculations.

During the summer of 1993, the Principal Investigator and an undergraduate student, Felecia Shaw, went to Lawrence Berkeley Laboratory where they worked with Arlon Hunt, Mary Quinby-Hunt, and Daniel Shapiro. They used a polarization-modulated nephelometer to measure the Mueller matrix elements from samples of two differently shaped objects. One sample was a suspension in distilled water of bacterial spores. The second sample consisted of latex spheres with a size parameter comparable to the bacterial spores. Measurements of the matrix elements were made at two wavelengths, 488 nm and 633 nm.

Results in 1994

Comparisons of Mie calculations with coupled-dipole (C-D) calculations for a sphere indicate that, with current computer limitations, the largest particle that can be modeled successfully has a length not greater than one micron. Examples of collections of helices, cylinders, ellipsoids, or cubes in that size range to validate the C-D calculations for non-spherical particles are difficult to find. However, we have made experimental measurements, or have located in the literature, experimental measurements of Mueller matrix elements for collections of particles such as octopus sperm heads (helices), a common bacteria, E. Coli (cylinders), bacterial spores (ellipsoids), and dried sea salt crystals (cubes). Experimental measurements of the Mueller matrix elements show some qualitative agreement with C-D calculations in each sample, but in general, the agreement is poor. A particle size distribution in each sample complicated the comparison of experimental measurement with C-D calculations. Furthermore, the larger particles in each collection exceed the size limitations of the C-D model.

It is clear at this point that until additional experimental data is available for non-spherical particles, the value of the coupled-dipole approximation method as a tool for predicting light scattering cannot be properly assessed. For this reason, future plans for this project include an experimental component.

Accomplishments in 1994

We have made considerable progress toward developing a practical model of polarized light scattering from non-spherical particles. Calculations of Mueller matrix elements have been made for single particles and collections of randomly oriented spheres, helices, cubes, ellipsoids and cylinders. Comparisons of the results of the calculations were made with experimental results and with Mie calculations. Mie calculations, which are less computer intensive than the coupled-dipole approximation, have been shown to accurately predict the scattering for marine organisms that are nearly spherical. Comparisons of the results of Mie calculations with those obtained using the coupled-dipole approximation in the limit as an ellipsoidal object approached a sphere helps to establish the limits of applicability of the Mie theory to non-spherical particles.

Publications/Technical Reports

PI - Shapiro, D.B., Hull, P.G., Hearst, J.E., and Hunt, A.J., 1993: Calculations of the Mueller scattering matrix for a DNA Plectonemic Helix, in preparation for J. Chem. Phys.

PI - Shapiro, D.B., Hull, P.G., Hunt, A.J., Shi, Y., McClain, W.M., Maestre, M.F., Quinby-Hunt, M.S., Hearst, J.E. 1993: Determination of the Average Orientation of DNA in the Octopus Sperm, Eledone cirrhosa using Polarized Light Scattering, submitted to Appl. Opt.

PS - Shapiro, D.B., Hull, P.G., Hunt, A.J., Shi, Y., Maestre, M.F., Quinby-Hunt, M.S., Hearst, J.E. 1993: Towards a working theory of polarized light scattering from helices, accepted by J. Chem. Phys.

Influences

1. Bohren, C. and Huffman, D. 1970: Absorption and Scattering of Light by Small Particles, Wiley, New York, NY.

2. Kattawar, G. and Adams, C. 1989: Stokes Vector Calculations of the Submarine Light Field in an Atmosphere-Ocean with Scattering According to a Rayleigh Phase Matrix: Effect of Interface Refractive Index on Radiance and Polarization, Limnol. Oceanogr., 34, 1453-1472.

3. Kattawar, G. 1990: Errors in Radiance Calculations by Using Scalar Rather than Stokes Vector Theory in a Realistic Atmosphere-Ocean System, Ocean X, Proc. SPIE, 1302-1312.

4. Purcell , E.M. and Pennypacker, C.R. 1973: Scattering and Absorption of Light by Non spherical Dielectric Grains, Astrophy. J. Vol.186, 705.

5. Singham, M., Singham, S. and Salzman, G. 1986: The scattering matrix for randomly oriented particles, J. Chem. Phys. 85, 3807.

Statistics

0 Papers published, refereed journals
2 Papers submitted, refereed journals
0 Books or chapters published, refereed publication
0 Books or chapters submitted, refereed publication
0 Invited presentations
0 Contributed presentations
0 Technical reports and papers, non-refereed journals
3 Undergraduate students supported
1 Graduate students supported
0 Post-docs supported
0 Other professional personnel supported

EEO/Minority Support
0 Female grad students
0 Minority grad students
1 Asian grad students
0 Female post-docs
0 Minority post-docs
0 Asian post-docs

Patents and awards
0